COARSENING OF FRACTAL INTERFACES

P. STREITENBERGER

Institut für Experimentelle Physik, Abteilung Materialphysik, Otto-von-Guericke-Universität Magdeburg, PSF 4120, D-39016 Magdeburg, Germany

The process of coarsening by curvature driven interface motion of fractal interfaces in two-dimensional space is studied by analytical and numerical methods. A statistical model is presented, which allows an analytical treatment of the main features of coarsening of a fractal interface. For non-conserved motion the interface is described by a statistical distribution function of size scales, which obeys a continuity equation in size space. The solution of the continuity equation yields, for a self-similar initial distribution function, the time development of the interface in terms of a time dependent size distribution function, which exhibits a growing lower characteristic length scale and leads to a power-law decay of the total interface length. The effect of coarsening on the scale of observation is discussed.

1 Introduction

Coarsening is a long-time relaxation phenomenon that is connected with an increase in the characteristic size scale of an unstable two- or multiphase microstructure. The driving force for this scale coarsening is the reduction of the excess free energy associated with the interface between different phases. The interface density $S_V = S/V$, i.e. the interface area S per unit volume V, decreases with time and therefore the characteristic size scale of the interface system given by $l = 1/S_V$ increases, the microstructure coarsens. For sufficiently long times the decrease in the interface density obeys the asymptotic power-law $S_V \approx t^{-\alpha}$, where for sufficiently smooth interfaces the coarsening exponent α only depends on the transport mechanism that drives the interface motion. For curvature driven interface motion (interface limited coarsening), as it is the case for antiphase domain coarsening [1] and normal grain growth [2, 3], the kinetic exponent has the universal value $\alpha = 1/2$ (parabolic growth law). In the case of diffusion limited coarsening the exponent is $\alpha = 1/3$ (Ostwald ripening [2, 4]). For interface limited coarsening the local order-parameter of the phase-ordering dynamics associated with the interface motion is non-conserved, while for diffusion limited coarsening the local order-parameter is conserved [5].

Recently there has been a great deal of interest in the coarsening kinetics of fractal structures. While the generation of fractal patterns far from equilibrium has been widely studied (cf. e.g. [6]), for the reverse process, the decay of a fractal structure, much less work has been done. In complex nonequilibrium systems such as fractal interfaces and clusters the dynamic power law is characterized by a non-trivial coarsening exponent. For the non-conserved curvature driven interface motion it has been shown theoretically as well as experimentally [7 to 10] that initially fractal interfaces exhibit a power law decay with a coarsening exponent α that depends on the fractal dimension. Although similar results has been found, by computer simulation, for the conserved coarsening dynamics of fractal clusters [11 to 13], a complete theoretical description is still lacking for this case [13].

However, also in the case of non-conserved fractal interface coarsening [7 to 10] no exact solution is available because the equation of motion of complex interfaces is highly nonlinear and can, in general, be solved only numerically. Therefore, Toyoki and Honda [7] used a scaling hypothesis to find the asymptotic power law for the coarsening of a non-random self-similar interface. They found for the coarsening exponent the relation $\alpha = (D+1-d)/2$, where D is the fractal dimension of the interface and d the Eucleadian dimension of the space. The same result was derived by Orihara and Ishibashi [8], however for a random fractal interface without assuming the self-similar evolution using a diffusion equation for the description of the interface motion. We could confirm the decay law by experimental observation [9, 10] and by a Monte Carlo simulation of the smoothing kinetics of initially fractal two-dimensional grain boundaries [10].

In the present paper a quite different approach is used to describe the coarsening process of a random self-similar interface. The random interface is described by a statistical distribution function of size scales or curvature radii, which obeys a continuity equation in size or curvature space. The solution of the continuity equation yields for non-conserved motion and an initial fractal distribution function the time development of the interface in terms of a time dependent size distribution function, which exhibits a growing lower characteristic length scale. Besides the description of the main features of the coarsening process this approach is also of physical interest because it is an example of how a cutoff of a statistical fractal may emerge in a complex system.

The paper is organized as follows. In order to give an illustrative insight into the coarsening process under consideration, in chapter 2 the dynamic scaling hypothesis and its confirmation (within the range of a lower and upper cutoff) by a Monte Carlo simulation is shortly discussed. In chapter 3 the statistical model is developed which allows for a simple initially random self-similar interface system an analytical solution in terms of a time dependent size distribution function. A summary concludes the paper.

2 Scaling Hypothesis and Monte Carlo Simulation

In general it is not possible to solve the equations of motion of the interface analytically due to the complexity of fractal interfaces in conjunction with the high nonlinearity of the equations of interface motion [7, 8]. Therefore the scaling hypothesis, after which the interface keeps self-similar during temporal evolution, may serve as a simple coarsening scenario [7, 9, 10, 11]. If we restrict ourselves to a plane section of an otherwise three-dimensional interface system the interface density is proportional to the total length L of the boundary line measured on the plane section of area A [9, 10]. For a non-random fractal boundary with a fractal dimension D_S ($1 \le D_S \le 2$), the boundary length obeyes the scaling relation

$$L \approx R_m^{-(D_S-1)}, \tag{1}$$

where R_m is the characteristic length of the structural unit of the boundary corresponding to the lower cutoff length of the fractal. The main effect of coarsening arises from the growth of the lower cutoff due to the time law

$$R_m \approx t^{\frac{1}{\beta+1}}, \tag{2}$$

where $\beta = 1$ for interface limited and $\beta = 2$ for diffusion limited growth. If we assume that the scaling relation Eq. (1) remains valid also during the relaxation process, the boundary length and therewith the interface density decreases as

$$L \approx t^{-\frac{D_S-1}{\beta+1}}. \tag{3}$$

For the case of non-conserved interface motion ($\beta = 1$) we have tested the decay law Eq. (3) by performing a Monte Carlo simulation of the thermal relaxation of initially fractal two-dimensional grains [10].

Using the Monte Carlo procedure described by Anderson et. al. [14] for modelling normal grain growth, a single closed grain is mapped onto a discrete square lattice of 512×512 lattice sites, where each lattice site is assigned the orientation number 1 or 2. The interface is defined to lie between two sites of unlike orientations. Taking only an interaction between nearest neighbours into account, the interface motion is simulated by employing a standard Monte Carlo technique in conjunction with an energy criterion for successful transition to the other orientation.

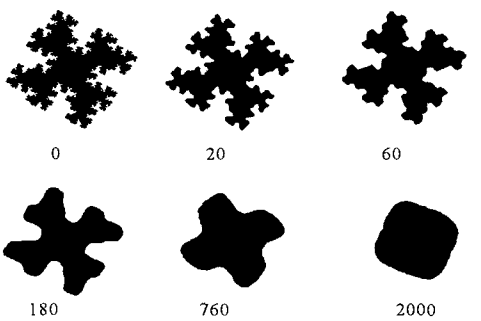

Figure 1: Simulation of the coarsening and shrinking process of an initially non-random fractal (D_S = 1.5).The numbers represent the time in Monte Carlo steps.

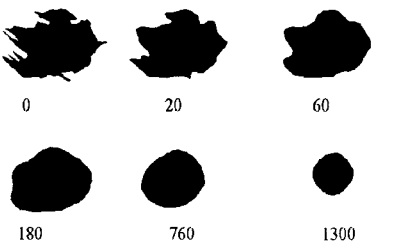

Figure 2: Same as for Fig. 1 but for an initially random shaped interface (D_S = 1.22) from a metallographic section of a deformed Zn specimen.

Figure 1 shows the simulation of the relaxation (and shrinking) process of an initially non-random fractal interface, the so-called square Koch-island (D_S = 1.5). The picture shows that the simulation clearly confirms , within a certain range between the lower and upper cutoff, the above scaling assumption that the boundary smoothens out step by step

from the higher to about the next lower generation of the initially self-similar fractal pattern. A similar simulation is shown in Fig. 2 starting with an irregularly shaped interface with an initial fractal dimension D_S = 1.22, which corresponds to a closed grain boundary from a metallographic section of a deformed Zn specimen (for details see [9, 10]).

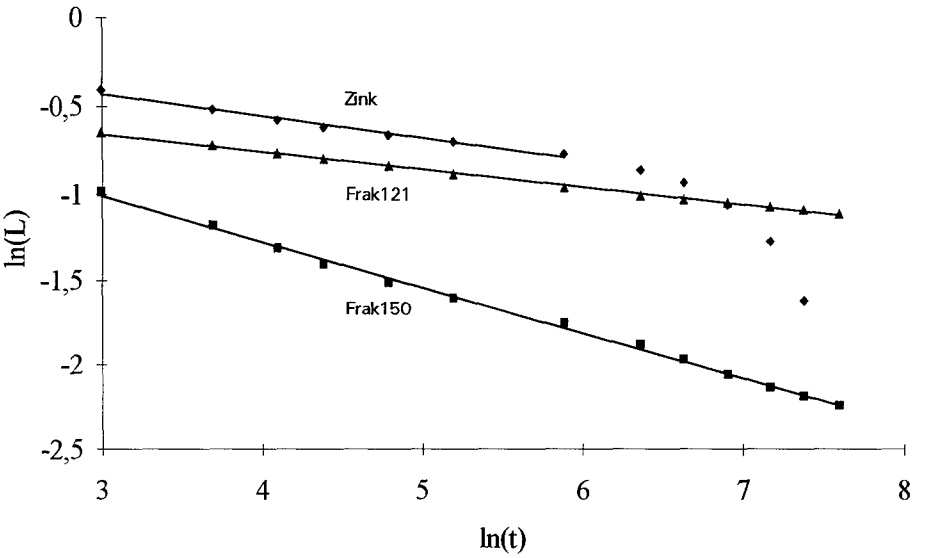

Figure 3: Plot of ln(L) versus ln(t) of the Monte Carlo simulation for three different fractal interfaces. The full lines represent the least-square fit to Eq. (3) ($\beta = 1$) (cf. Table I). L is normalized to the boundary length at $t = 0$.

The log-log plot of the boundary length L (perimeter) of the grains in Figs. 1 and 2 versus simulation time t (measured in Monte Carlo steps) in Fig. 3 shows that the coarsening kinetics, in fact, follows over a wide range the time law Eq. (3) for $\beta = 1$. The fractal dimension derived from the coarsening kinetics, i.e. from the slopes of the full lines in Fig. 3 via the time exponent (1 - D_S)/2 in Eq. (3) (for $\beta = 1$), agrees well with the fractal dimension determined by the geometry of the initial interface (Table I). For the random interface (Fig. 2), as time elapses, the crossover from self-similar boundary coarsening to normal grain shrinking kinetics governed by the parabolic time law L_0^2 - L^2 $\approx t$ can be observed in Fig. 3 [10].

In the following paragraph a statistical coarsening model for a much simpler interface configuration is presented, which allows, however, an analytical treatment beyond the above scaling hypothesis of all the main features of self-similar interface coarsening.

Table I: Fractal dimension of self-similar interfaces from the coarsening kinetics

	D_S (from the fractal geometry of the initial interface)	D_S (from the coarsening kinetics, Fig. 3 and Eq. (3))
Frak 150: square Koch island	1.50	1.54
Frak 121: modified Koch island	1.21	1.20
Zink: random interface	1.22 (yardstick method)	1.25

3 Statistical Model of Non-Conserved Coarsening of a Self-Similar Interface

In the following considerations we replace the complex fractal boundaries of the preceding paragraph by the somewhat simpler system of a two-dimensional random assembly of non-overlapping and non-interacting closed circular loops of different curvature radii R. For a non-conserved system the equation of motion for a single circular interface with radius R is given by

$$\dot{R} = -kK^{\beta} = -k\frac{1}{R^{\beta}}, \tag{4}$$

where $\dot{R}$ is the radial velocity, K the curvature and k the mobility of the interface. Again $\beta = 1$ for interface limited growth and $\beta = 2$ for diffusion limited growth. For the description of the time development of the total interface, i.e. of the whole assembly of circular loops, we introduce the size distribution function $F(R,t)$, where $F(R,t)dR$ gives the number of loops per unit area with radius between R and $R + dR$. For a random fractal interface the initial size distribution function is assumed to have the hyperbolic form

$$F(R,0) = F_0(R) = BR^{-D_S-1}, \tag{5}$$

where D_S is the fractal dimension of the whole assembly and B a constant. Since during coarsening no new loop is created and the only process of annihilation of interfaces is the shrinking of loops according to the growth law Eq. (4) the size distribution function must obey a continuity equation in size space given by

$$\frac{\partial F(R,t)}{\partial t} + \frac{\partial}{\partial R}\left(\dot{R}F(R,t)\right) = 0. \tag{6}$$

For a given initial distribution $F(R,0) = F_0(R)$ the solution of the first-order partial differential equation (6) can be written in the form [15]

$$F(R,t) = F_0\left(R_0(R,t)\right)\frac{\partial R_0(R,t)}{\partial R}, \tag{7}$$

where $R_0 = R_0(R,t)$ is the solution of the characteristic equation (4) with the integration constant $R_0 = R(t=0)$. The integration of Eq. (4) yields

$$R_0 = \left(R^{\beta+1} + (\beta+1)kt\right)^{\frac{1}{\beta+1}}. \tag{8}$$

Equations (5) and (8) inserted into Eq. (7) leads to the size distribution function

$$F(R,t) = BR^{\beta}\left(R^{\beta+1} + (\beta+1)kt\right)^{-\frac{\beta+D_S+1}{\beta+1}}. \tag{9}$$

At $t = 0$ Eq. (9) reduces to the initial distribution Eq. (5). At $t > 0$, in contrast to the

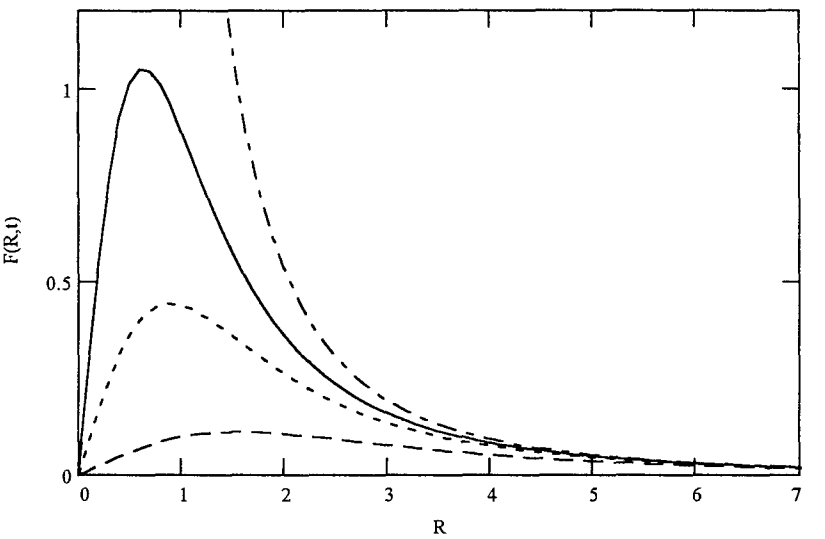

Figure 4: Size distribution function Eq. (9) for $\beta = 1$ and $D_S = 1.5$ at different times t. Dot-dashed line: $t = 0$ (initial distribution Eq. (5)), full line: $t_1 > 0$, dotted line: $t_2 = 2t_1$, dashed line: $t_3 = 6t_1$. R and t are given in terms of arbitrary unit length and unit time, respectively.

initial distribution function, $F(R,t)$ exhibits a maximum and tends towards zero for vanishing radius R (Fig. 4). The location of the maximum defines a natural characteristic

length scale or lower „cutoff" $R_m = R_m(t)$ where scaling breaks down:

$$R_m(t) = \left(\frac{k\beta(\beta+1)t}{D_S+1} \right)^{\frac{1}{\beta+1}} . \tag{10}$$

In the following discussion we restrict ourselves to interface limited coarsening ($\beta = 1$), where R_m increases with time as

$$R_m(t) = \left(\frac{2kt}{D_S+1} \right)^{1/2} . \tag{11}$$

The total number of loops decays as

$$N(t) = \int_0^\infty F(R,t)dR = \frac{B}{D_S}(2kt)^{-D_S/2} , \tag{12}$$

which is associated with a decrease in the total length of the interface

$$L(t) = 2\pi \int_0^\infty RF(R,t)dR = 2\pi B g(0,D_S)(2kt)^{-\frac{D_S-1}{2}} . \tag{13}$$

In this relation $g(0,D_S)$ is defined by the integral

$$g(x,D_S) = \int_x^\infty \xi^2 \left(\xi^2+1\right)^{-\frac{D_S+2}{2}} d\xi . \tag{14}$$

For the average radius we obtain

$$< R >= \frac{L(t)}{N(t)} = 2\pi g(0,D_S)(2kt)^{1/2} , \tag{15}$$

i.e. $< R > \approx R_m(t)$.

The power-law behaviour of the interface length Eq. (13) results in the present approach, without assuming the scaling hypothesis Eq. (1) during the temporal evolution, from the initial fractal distribution function in conjuntion with the growth law Eq.(4) and the continuity equation (6). While for a deterministic fractal the lower cutoff length is simply defined by the lower limit of the geometric building block, for the present statistical

fractal the lower characteristic length scale emerges from the physics of the coarsening process. The emergence of empirical random fractals limited by a lower and upper cutoff has been discussed from a different point of view also in [16].

The present model allows in a simple but instructive way to study the effect of coarsening on the resolution of the interface length by measurement. If we assume that for a certain measuring device the resolution of length scale is restricted to radii $R' \geq R$ the number of loops that can be observed by that device is given by

$$N(R,t) = \int_R^\infty F(R',t)dR' = \frac{B}{D_S}\left(R^2 + 2kt\right)^{-\frac{D_S}{2}} . \tag{16}$$

The total interface length that can be measured is

$$L(R,t) = 2\pi \int_R^\infty R'F(R',t)dR' = 2\pi B(2kt)^{-\frac{D_S-1}{2}} g(R/(2kt)^{1/2}, D_S) , \tag{17}$$

where the function $g(x, D_S)$ is defined by the integral Eq. (14).

Fig. 5 shows in form of a log-log plot the observable interface length Eq. (17) versus

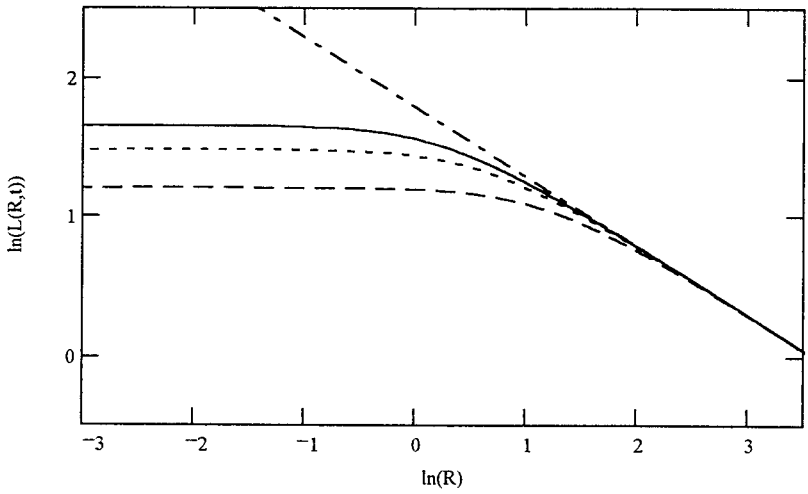

Figure 5: Log-log plot of the interface length Eq. (17) versus R at different times as in Fig. 4.

resolution, that is, in dependence of the segments of scale R that are needed to approximate the interface length (Richardson plot), at different times.

The coarsening, i.e. the growth of the lower characteristic length, leads to a reduction in the available scaling range at smaller R. The width of the crossover region from the eucleadian behaviour at small R to the fractal behaviour at large R becomes broader with increasing time.This behaviour can quantitatively be characterized by the slope of the curves in Fig. 5, or alternatively, by the effective fractal dimension [17]

$$D_{eff}(R,t) = 1 - \frac{d \ln L(R,t)}{d \ln R}, \tag{18}$$

which depends on the scale of observation R. $D_{eff} = D_{eff}(R,t)$ shows a crossover from $D_{eff} = 1$ at small R (high resolution) to $D_{eff} = D_S$ at large R (low resolution) (Fig. 6). For later times corresponding to a more relaxed interface, D_{eff} approaches D_S at larger R. This may have an effect on the empirical fractal dimension of the interface, which is obtained by application of an empirical observation method, as the yardstick or box counting method, at a fixed coarsening state.

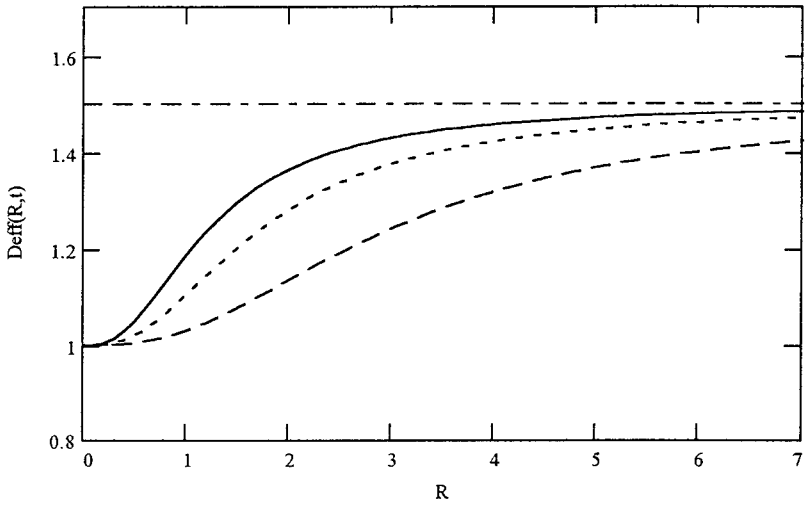

Figure 6: Scale dependent effective fractal dimension Eq. (18) at different times as in Fig. 4.

If we consider D_{eff} as an estimate for the empirical fractal dimension and if we take into account that for a sufficiently coarsened interface D_{eff} may remain well below the asymptotic value D_S in Fig. 6 because the usable scale of R is limited by the existence of an upper cutoff defined by the sample size (e.g. by the grain size in Fig. 1), it follows that the empirical fractal dimension decreases during coarsening. Hence, for each coarsening state of the grain in Fig. 1, for example, a somewhat lower empirical fractal dimension

than for the previous state might be found. In contrast, the corresponding coarsening kinetics, as represented by the slope of the straight lines in Fig. 3, is uniquely determined by the „initial" fractal dimension D_S that is inherent to the initial self-similar interface or, as in the present statistical model, to the initial distribution function Eq. (5).

Finally, it is worth noting that the functional form of the fractal equation (17) is quite different from Rigaut's empirical interpolation Ansatz [18] for concave log-log plots. Rigaut's interpolation formula has the form

$$L = c_1 (1 + c_2 R^{D_S - 1})^{-1}, \tag{19}$$

which tends in a log-log plot as Fig. 5 towards the horizontal maximum at high resolution and towards the ideal fractal at low resolution. From the limiting behaviour of Eq. (17) for small and large R one finds $c_1 = L(t)$ and $c_2 = (D_S - 1)L(t)/(2\pi B)$, respectively, where $L(t)$ is given by Eq. (13). A quantitative comparison shows that this interpolation formula represents only a poor approximation to the exact fractal equation (17) in the crossover region.

4 Summary

After a discussion of the dynamic scaling behaviour of self-similar interfaces as it follows from analytical scaling assumptions and numerical Monte Carlo simulations a statistical model was presented, which shows all the main features of coarsening of fractal interfaces. The coarsening kinetics of a two-dimensional non-conserved interface system consisting of a random assembly of non-interacting circular loops could be described by a size distribution function obeying a continuity equation in size space. For a self-similar initial distribution the solution of the continuity equation yielded a time dependent size distribution function, which exhibts a lower characteristic length scale where scaling breaks down. Physically this emerges from the curvature driven relaxational motion of the interfaces leading to parabolic growth of the characteristic length scale. The total interface length shows the characteristic power-law decay, where the coarsening exponent depends on the inherent fractal dimension of the initial interface. The model allowed us to calculate the interface length as a function of resolution, which led us to a discussion of the effect of coarsening on the scale of observation.

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